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Simulation of Neutron and Gamma Ray Emission from Fission

Fission Library Development Team

Lawrence Livermore National Laboratory

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1 Introduction

This paper describes a general-purpose and extensible software library to accurately simulate neutron and gamma-ray emission from fission reactions (both spontaneous and neutron induced). In a fission event, Monte-Carlo codes need to sample a number of distributions: the number of neutrons emitted in the fission, the energy of these neutrons, the number of gamma rays emitted in the fission, and the energy of these gamma rays. For a complete simulation, one should correlate the number of neutrons to the number of gamma rays, as well as the neutron and gamma ray energies. However, very little data is available for these correlations so the software module currently samples all of the distributions independently. Section 2 describes the data that is available from the literature for fission neutrons, and the model that the fission module has implemented. Section 3 deals with fission gamma-rays. The software library can be downloaded from `http://nuclear.llnl.gov/CNP/simulation`.

2 Neutrons emitted by fission

This section contains three parts. The first part is on induced fission neutron number distributions, the second part on spontaneous fission neutron number distribution while the third part is on neutron spontaneous and induced fission energy spectra.

2.1 Induced fission neutron number distribution

Zucker and Holden [2] measured the P_ν distributions for ^{235}U, ^{238}U, and ^{239}Pu (see tables 1, 2, 3), as a function of the energy E_n of the fission inducing neutron for 0 through 10 MeV in increments of a 1 MeV. Fig. 1 shows the neutron number distribution for induced fission of ^{235}U.

By fitting that data, Valentine [3] [4] expressed the P_ν's (for $\nu = 0, ..., 8$) as a function of the energy E_n. The functions $P_\nu(E_n)$ can then be used to sample the neutron multiplicity when the energy E_n of the incident neutron is not among the energies tabulated by Zucker and Holden. When E_n is greater than 10 MeV, E_n=10 MeV is used to generate P_ν. The module uses the data in that manner when the 'nudist' option is set to 0.

Gwin, Spencer and Ingle [5] measured the P_ν distribution at thermal energies for ^{235}U. This data was used to generate modified $P_\nu(E_n)$ distributions that can be exercised when the 'nudist' option is set to 1 in the fission module. Again, when E_n is greater than 10 MeV, E_n=10 MeV is used to generate P_ν.

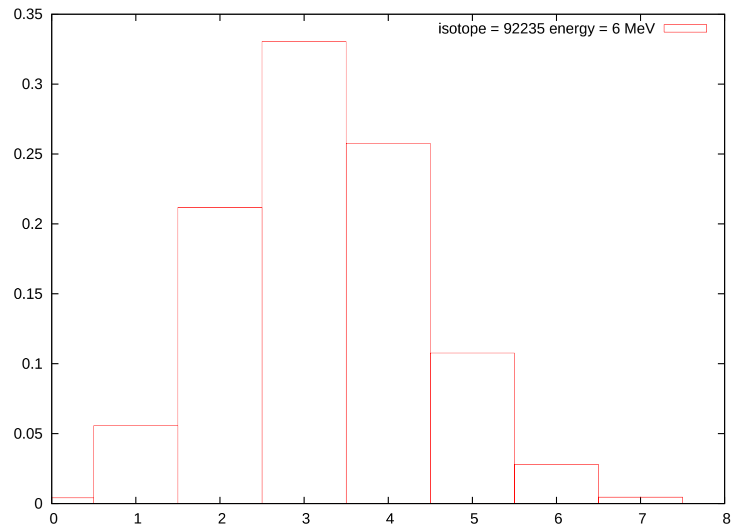

Figure 1: Induced fission in ^{235}U, incident neutron energy = 6MeV

E_n	ν=0	1	2	3	4	5	6	7
0	.0317223	.1717071	.3361991	.3039695	.1269459	.0266793	.0026322	.0001449
1	.0237898	.1555525	.3216515	.3150433	.1444732	.0356013	.0034339	.0004546
2	.0183989	.1384891	.3062123	.3217566	.1628673	.0455972	.0055694	.0011093
3	.0141460	.1194839	.2883075	.3266568	.1836014	.0569113	.0089426	.0019504
4	.0115208	.1032624	.2716849	.3283426	.2021206	.0674456	.0128924	.0027307
5	.0078498	.0802010	.2456595	.3308175	.2291646	.0836912	.0187016	.0039148
6	.0046272	.0563321	.2132296	.3290407	.2599806	.1045974	.0265604	.0056322
7	.0024659	.0360957	.1788634	.3210507	.2892537	.1282576	.0360887	.0079244
8	.0012702	.0216090	.1472227	.3083032	.3123950	.1522540	.0462449	.0107009
9	.0007288	.0134879	.1231200	.2949390	.3258251	.1731879	.0551737	.0135376
10	.0004373	.0080115	.1002329	.2779283	.3342611	.1966100	.0650090	.0175099

Table 1: Neutron number distribution for induced fission in ^{235}U

Instead of fitting the P_ν distributions as a function of E_n with a least-square polynomial, Valentine [3] used the observation made by Frehaut [6] that a unique relationship $P_\nu(\overline{\nu})$ for each ν could sufficiently well capture the multiplicity distributions of a number of major isotopes. This distribution is expressed as a function of the average number of neutrons emitted $\overline{\nu}$. Based on that observation, the P_ν distributions are least-square fitted as a function of $\overline{\nu}$ instead of E_n in Valentine's work. The fit to the ^{235}U data is used for both ^{235}U and ^{233}U neutron induced fission, the fit to ^{238}U for ^{232}U, ^{234}U, ^{236}U and ^{238}U, while the fit to ^{239}Pu for ^{239}Pu and ^{241}Pu. The fits are only used when $\overline{\nu}$ is in the range of the $\overline{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation (see below) is used. The fission module uses these fits when the 'nudist' option is set to 2.

The fourth way of sampling the Zucker and Holden multiplicity distributions is similar to the one above based on the observation by Frehaut, in that the multiplicity data for one isotope is used for other isotopes. However it differs from it in that the P_ν distributions are not least-square fitted as a function of $\overline{\nu}$, but are left intact as 11 multiplicity distributions for each of the 11 energies listed in Zucker and Holden. The

E_n	ν=0	1	2	3	4	5	6	7	8
0	.0396484	.2529541	.2939544	.2644470	.1111758	.0312261	.0059347	.0005436	.0001158
1	.0299076	.2043215	.2995886	.2914889	.1301480	.0363119	.0073638	.0006947	.0001751
2	.0226651	.1624020	.2957263	.3119098	.1528786	.0434233	.0097473	.0009318	.0003159
3	.0170253	.1272992	.2840540	.3260192	.1779579	.0526575	.0130997	.0013467	.0005405
4	.0124932	.0984797	.2661875	.3344938	.2040116	.0640468	.0173837	.0020308	.0008730
5	.0088167	.0751744	.2436570	.3379711	.2297901	.0775971	.0225619	.0030689	.0013626
6	.0058736	.0565985	.2179252	.3368863	.2541575	.0933127	.0286200	.0045431	.0031316
7	.0035997	.0420460	.1904095	.3314575	.2760413	.1112075	.0355683	.0065387	.0031316
8	.0019495	.0309087	.1625055	.3217392	.2943792	.1313074	.0434347	.0091474	.0046284
9	.0008767	.0226587	.1356058	.3076919	.3080816	.1536446	.0522549	.0124682	.0067176
10	.0003271	.0168184	.1111114	.2892434	.3160166	.1782484	.0620617	.0166066	.0095665

Table 2: Neutron number distribution for induced fission in ^{238}U

E_n	ν=0	1	2	3	4	5	6	7	8
0	.0108826	.0994916	.2748898	.3269196	.2046061	.0726834	.0097282	.0006301	.0001685
1	.0084842	.0790030	.2536175	.3289870	.2328111	.0800161	.0155581	.0011760	.0003469
2	.0062555	.0611921	.2265608	.3260637	.2588354	.0956070	.0224705	.0025946	.0005205
3	.0045860	.0477879	.1983002	.3184667	.2792811	.1158950	.0301128	.0048471	.0007233
4	.0032908	.0374390	.1704196	.3071862	.2948565	.1392594	.0386738	.0078701	.0010046
5	.0022750	.0291416	.1437645	.2928006	.3063902	.1641647	.0484343	.0116151	.0014149
6	.0014893	.0222369	.1190439	.2756297	.3144908	.1892897	.0597353	.0160828	.0029917
7	.0009061	.0163528	.0968110	.2558524	.3194566	.2134888	.0729739	.0213339	.0020017
8	.0004647	.0113283	.0775201	.2335926	.3213289	.2356614	.0886183	.0274895	.0039531
9	.0002800	.0071460	.0615577	.2089810	.3200121	.2545846	.1072344	.0347255	.0054786
10	.0002064	.0038856	.0492548	.1822078	.3154159	.2687282	.1295143	.0432654	.0075217

Table 3: Neutron number distribution for induced fission in ^{239}Pu

multiplicity distribution P_ν from which the number of neutrons will be sampled is selected based on the value of $\bar{\nu}$ entered for a given induced fission event. For instance, if $P_\nu(1)$ for 1 MeV has $\bar{\nu} = 2.4$, $P_\nu(2)$ for 2 MeV has $\bar{\nu} = 2.6$, and $\bar{\nu}$ is 2.45 at the energy of the incident fission-inducing neutron (this value $\bar{\nu}$ comes typically from cross-section data libraries such and ENDF/ENDF), the probability of sampling the number of neutrons ν from $P_\nu(1)$ and $P_\nu(2)$ will be 25% and 75%, respectively. This technique is only used when $\bar{\nu}$ is in the range of the $\bar{\nu}$'s for the tabulated data. Otherwise, Terrell's approximation (see below) is used. This last way of computing ν has several advantages: first, the data as listed in the original paper is used exactly, as opposed to approximated by low-ordered polynomials least-square fitting the original data. Second, the data from the Zucker and Holden paper is entered as-is as a table in the code, and can easily be checked and maintained if necessary by the application developer. Third the method provides a simple and statistically correct mechanism of sampling the Zucker and Holden tables. The fission module behaves in this manner when the 'nudist' option is set to 3, which is also the default behavior.

Terrell [1] showed, on reasonable assumptions as to the distribution of excitation energy among fission fragments, that the probability P_ν of observing ν neutrons from fission are given approximately, in cumulative form, by the "Gaussian" distribution,

$$\sum_{n=0}^{\nu} P_n = \frac{1}{2\pi} \int_{-\infty}^{\frac{\nu-\bar{\nu}+\frac{1}{2}+b}{\sigma}} e^{-\frac{t^2}{2}} dt \tag{1}$$

In this equation, $\bar{\nu}$ is the average number of neutrons, b is a small correction factor $b < 0.01$ to ensure that the ν's are positive, while σ is equal to 1.079. Terrell showed that this expression can be used for several different isotopes, and this is the one that the fission module will be using by default for isotopes where no data is available.

2.2 Spontaneous fission neutron number distribution

For ^{252}Cf, the fission module can be set to use either the measurements by Spencer [7] (ndist set to 0), or the distributions by Boldeman [8] (ndist set to 1).

For ^{238}U, ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{242}Cm, ^{244}Cm, the probability distribution data comes from Holden and Zucker [10]. The measured data is summarized in table 4.

isotope	ν=0	1	2	3	4	5	6	7	8	9
^{238}U	.0481677	.2485215	.4253044	.2284094	.0423438	.0072533	0	0	0	0
^{238}Pu	.0540647	.2053880	.3802279	.2248483	.1078646	.0276366	0	0	0	0
^{242}Pu	.0679423	.2293159	.3341228	.2475507	.0996922	.0182398	.0031364	0	0	0
^{242}Cm	.0212550	.1467407	.3267531	.3268277	.1375090	.0373815	.0025912	.0007551	.0001867	0
^{244}Cm	.0150050	.1161725	.2998427	.3331614	.1837748	.0429780	.0087914	.0002744	0	0
^{252}Cf [7]	.00211	.02467	.12290	.27144	.30763	.18770	.06770	.01406	.00167	.0001
^{252}Cf [8]	.00209	.02621	.12620	.27520	.30180	.18460	.06680	.01500	.00210	0

Table 4: Neutron number distribution for spontaneous fission

If no full multiplicity distribution data exists, the fission module uses Terrell [1]'s approximation with $\bar{\nu}$ from Ensslin [9]. Ensslin has $\bar{\nu}$ data for the isotopes in table 5.

isotope	$\bar{\nu}$
^{232}Th	2.14
^{232}U	1.71
^{233}U	1.76
^{234}U	1.81
^{235}U	1.86
^{236}U	1.91
^{238}U	2.01
^{237}Np	2.05
^{238}Pu	2.21
^{239}Pu	2.16
^{240}Pu	2.156
^{241}Pu	2.25
^{242}Pu	2.145
^{241}Am	3.22
^{242}Cm	2.54
^{244}Cm	2.72
^{249}Bk	3.40
^{252}Cf	3.757

Table 5: Average number of neutrons per spontaneous fission

2.3 Spontaneous and induced fission neutron energy distribution

All of the fission spectra in the Evaluated Nuclear Data Library, ENDL [11] are defined by a simple analytical function, a Watt spectrum defined as

$$W(a,b,E') = Ce^{-aE'} sinh(\sqrt{bE'}) \tag{2}$$

where $C = \sqrt{\pi \frac{b}{4a} \frac{e^{\frac{b}{4a}}}{a}}$, and E' is the secondary neutron energy. The Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV is shown in Fig. 2.

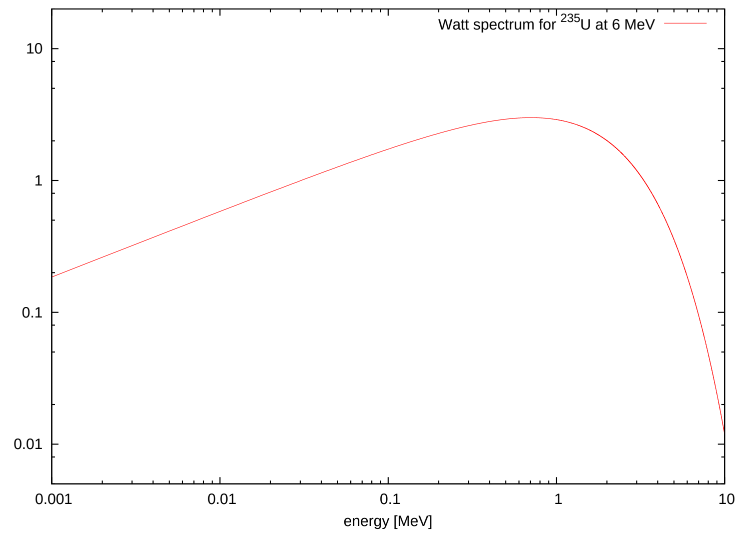

Figure 2: Watt spectrum for ^{235}U and an incident neutron energy of 6 MeV

The coefficients a and b vary weakly from one isotope to another and also vary weakly with the incident neutron energy. In the fission module, b is set identical to 1.0, and a is parametrized as a simple function of the incident neutron energy, as implemented in TART [14, 12]. The fissioning isotope and incident neutron energy determine the value of a, and the energy E' of the secondary neutron emitted is sampled using the Los Alamos' Monte Carlo sampler attributed to Mal Kalos [13].

The Watt spectrum is used for all isotopes but ^{252}Cf, for which a special treatment summarized by Valentine [3] is applied. The neutron spectrum for ^{252}Cf is sampled from either the Mannhart [15] corrected Maxwellian distribution ('neng' set to 0, default), the Madland and Nix [16] ('neng' set to 1), or the Watt fission spectra from Froehner [17] ('neng' set to 2).

3 Gammas emitted by fission

This section contains three parts. The first part is on fission gamma ray number distributions, the second part is on fission gamma ray energy spectrum.

3.1 Spontaneous and induced fission gamma ray number distribution

The fission module uses Brunson [18]'s double Poisson model for the spontaneous fission gamma ray multiplicity of ^{252}Cf (see Fig. 3).

$$\Pi(G) = 0.682\frac{7.20^G e^{-7.20}}{G!} + 0.318\frac{10.71^G e^{-10.72}}{G!} \tag{3}$$

where G is the gamma ray multiplicity.

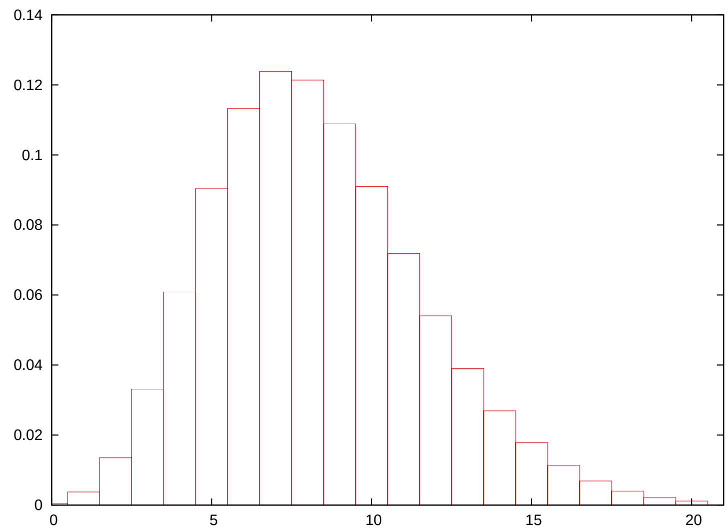

Figure 3: Fission gamma-ray multiplicity for ^{252}Cf

The prompt gamma ray multiplicity ranges from 0 to 20 gama rays per fission with an average of 8.32 gamma rays per fission. This model is a fit to experimental data measured by Brunson himself.

For other isotopes, there is no data available for the multiplicity of prompt gamma rays. Valentine [19] used an approximation that was adopted by the fission module. The probability of emitting G fission gamma rays obeys the negative binomial distribution:

$$\Pi(G) = \left(\begin{array}{c} \alpha + G - 1 \\ G \end{array} \right) p^G (1-p)^G \tag{4}$$

where the parameter p can be written as $p = \frac{\alpha}{\alpha + \bar{G}}$, α is approximately 26 and $\bar{G}$ is the average number of gamma rays per fission. $\bar{G}$ is approximated by

$$\bar{G} = \frac{E_t(\bar{\nu},Z,A)}{E} \tag{5}$$

where $E_t(\bar{\nu},Z,A) = (2.51(\pm 0.01) - 1.13 \cdot 10^{-5}(\pm 7.2 \cdot 10^{-8})Z^2\sqrt{A})\nu + 4.0$ is the total prompt gamma ray energy, and $\bar{E} = -1.33(\pm 0.05) + 119.6(\pm 2.5)\frac{Z^{\frac{1}{3}}}{A}$ is the average prompt gamma ray energy. The multiplicity distribution for the spontaneous fission of ^{238}U is shown in Fig. 4.

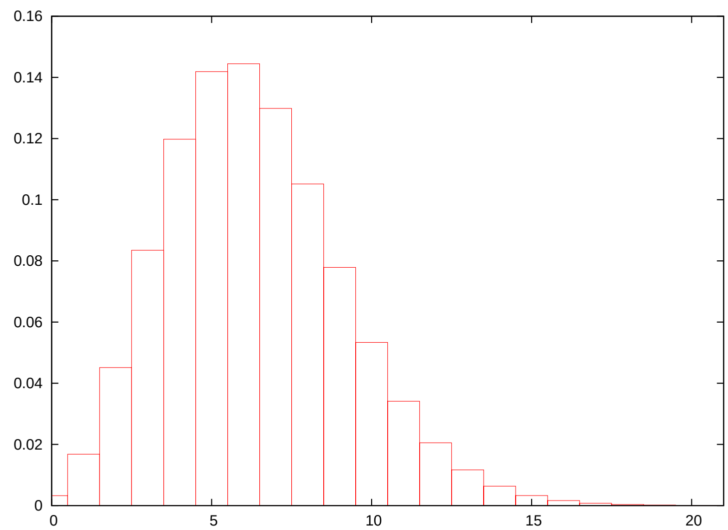

Figure 4: Fission gamma-ray multiplicity for spontaneous fission of ^{238}U

These multiplicity distributions are only estimates and are not measured data. The fission module uses this model for estimating the number of gamma rays from both spontaneous and induced fission.

3.2 Spontaneous and induced fission gamma ray energy distribution

The fission module implements Valentine's [3] model for the energy spectra of fission gamma-rays. The only measured energy spectra for fission gamma-rays are for the spontaneous fission of ^{252}Cf and for the termal-neutron-induced fission of ^{235}U. Both spectra are similar [20]. Because the ^{235}U measurements are more precise, this data will be used for the fission gamma-ray spectrum. The energy spectrum of the prompt fission gamma rays is obtained from Maienschein's measurements [21] [22]:

$$N(E) = 38.13 * (E - 0.085)e^{1.648E} for E < 0.3MeV \tag{6}$$

$$N(E) = 26.8e^{-2.30E} for 0.3 < E < 1.0MeV \tag{7}$$

$$N(E) = 8.0e^{-1.10E} for 1.0 < E < 8.0MeV \tag{8}$$

This probability function is shown in Fig. 5. Because gamma ray energy spectra are not available, the spectrum above is used for all isotopes, both for spontaneous and induced fissions.

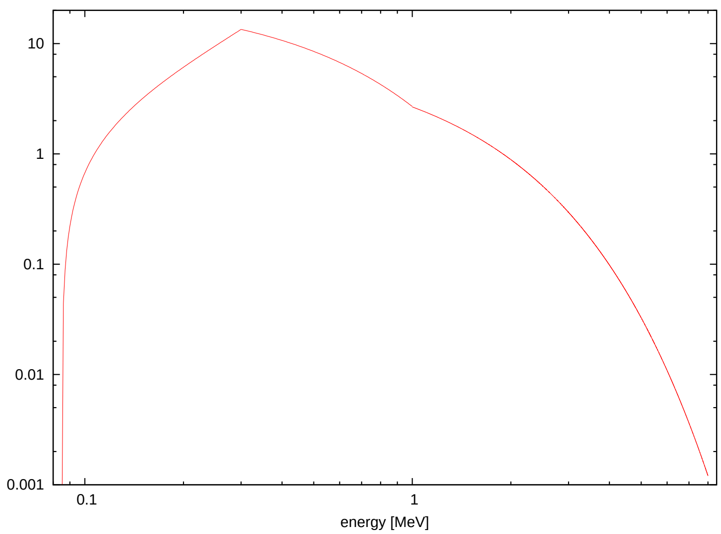

Figure 5: Fission gamma-ray spectrum for ^{235}U

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